

APPROXIMATIONS FOR THE CAPUTO DERIVATIVE (II)

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Abstract

In this paper we use the Fourier transform method and the expansion formula for the polylogarithm function to derive approximations for the Caputo derivative of order $2-\alpha$ and 2. The approximations are applied for computing the numerical solutions of the fractional relaxation and subdiffusion equations. While the properties of the weights of the approximation of order $2-\alpha$ are similar to those of the $L1$ approximation, the corresponding numerical solution is more accurate for the examples discussed in the paper and many of the functions used in practice.

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1 Introduction

Approximations of fractional integrals and derivatives have recently been an active research topic [5, 8, 9, 19, 21, 24, 27]. The fractional integral of order $\alpha > 0$ and the Caputo derivative of order α , where $0 < \alpha < 1$ are defined as

$$I^\alpha y(x) = \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} y(t) dt,$$

$$y^{(\alpha)}(x) = D^\alpha y(x) = \frac{1}{\Gamma(1-\alpha)} \int_0^x \frac{y'(t)}{(x-t)^\alpha} dt.$$

Let $h = x/n$, where n is a positive integer, and $x_m = mh$, $y_m = y(x_m)$. The $L1$ approximation (1) for the Caputo derivative is a commonly used approximation for numerical solution of fractional differential equations.

$$y_n^{(\alpha)} = \frac{1}{\Gamma(2-\alpha)h^\alpha} \sum_{k=0}^n \sigma_k^{(\alpha)} y_{n-k} + O(h^{2-\alpha}), \quad (1)$$

where $\sigma_0^{(\alpha)} = 1$, $\sigma_n^{(\alpha)} = (n-1)^{1-\alpha} - n^{1-\alpha}$ and

$$\sigma_k^{(\alpha)} = (k+1)^{1-\alpha} - 2k^{1-\alpha} + (k-1)^{1-\alpha}, \quad (k = 2, \dots, n-1).$$

The weights $\sigma_k^{(\alpha)}$ of the $L1$ approximation have the following properties

$$\begin{aligned} \sigma_0^{(\alpha)} > 0, \quad \sigma_1^{(\alpha)} < \sigma_2^{(\alpha)} < \dots < \sigma_k^{(\alpha)} < \dots < \sigma_{n-1}^{(\alpha)} < 0, \quad \sigma_n^{(\alpha)} < 0, \\ \sum_{k=0}^n \sigma_k^{(\alpha)} = 0, \quad \sum_{k=1}^n k \sigma_k^{(\alpha)} = -n^{1-\alpha}, \\ \sigma_k^{(\alpha)} = \frac{C_1}{k^{1+\alpha}} + O\left(\frac{1}{k^{2+\alpha}}\right), \quad \sigma_n^{(\alpha)} = \frac{C_2}{n^\alpha} + O\left(\frac{1}{n^{1+\alpha}}\right), \end{aligned} \quad (2)$$

where $C_1 = \alpha(\alpha-1)$ and $C_2 = \alpha-1$. When the function y has a continuous second derivative, the $L1$ approximation has accuracy $O(h^{2-\alpha})$ ([17]). The numerical solution of the fractional relaxation equation (20) which uses the $L1$ approximation for the Caputo derivative is computed with [5]

$$u_n = \frac{1}{\sigma_0^{(\alpha)} + \Gamma(2-\alpha)h^\alpha} \left(\Gamma(2-\alpha)h^\alpha F_n - \sum_{k=1}^n \sigma_k^{(\alpha)} u_{n-k} \right), \quad u_0 = y_0. \quad (3)$$

In Table 1 we compute the error and the order of numerical solution (3) for Equation I and $\alpha = 0.25$, Equation II and $\alpha = 0.5$ and Equation III, $\alpha = 0.75$. In [5] we derived the second-order expansion of the $L1$ approximation

$$\frac{1}{\Gamma(2-\alpha)h^\alpha} \sum_{k=0}^n \sigma_k^{(\alpha)} y(x-kh) = y^{(\alpha)}(x) + \frac{\zeta(\alpha-1)}{\Gamma(2-\alpha)} y''(x) h^{2-\alpha} + O(h^2).$$

By approximating $y''(x)$ using second-order backward difference we obtain the second-order approximation for the Caputo derivative

$$y_n^{(\alpha)} = \frac{1}{\Gamma(2-\alpha)h^\alpha} \sum_{k=0}^n \delta_k^{(\alpha)} y_{n-k} + O(h^2), \quad (4)$$

Table 1: Maximum error and order of numerical solution (3) of Equation I and $\alpha = 0.25$, Equation II and $\alpha = 0.5$ and Equation III with $\alpha = 0.75$.

h	Equation I		Equation II		Equation III	
	Error	Order	Error	Order	Error	Order
0.003125	0.0000466	1.6970	0.0000513	1.4857	0.0024184	1.2442
0.0015625	0.0000143	1.7071	0.0000183	1.4901	0.0010191	1.2468
0.00078125	4.3×10^{-6}	1.7150	6.5×10^{-6}	1.4931	0.0004290	1.2482
0.000390625	1.3×10^{-6}	1.7212	2.3×10^{-6}	1.4952	0.0001805	1.2490

where $\delta_k^{(\alpha)} = \sigma_k^{(\alpha)}$ for $2 \leq k \leq n$ and

$$\delta_0^{(\alpha)} = \sigma_0^{(\alpha)} - \zeta(\alpha - 1), \quad \delta_1^{(\alpha)} = \sigma_1^{(\alpha)} + 2\zeta(\alpha - 1), \quad \delta_2^{(\alpha)} = \sigma_2^{(\alpha)} - \zeta(\alpha - 1).$$

The weights $\delta_k^{(\alpha)}$ of approximation (4) satisfy

$$\delta_0^{(\alpha)} > 0, \quad \delta_1^{(\alpha)} < 0, \quad \delta_2^{(\alpha)} > 0, \quad \delta_3^{(\alpha)} < \delta_4^{(\alpha)} < \dots < \delta_k^{(\alpha)} < \dots < \delta_{n-1}^{(\alpha)} < 0.$$

The asymptotic expansions of the trapezoidal approximation for the definite integral and the integral approximations for the fractional derivative involve the values of the *Riemann zeta function* defined as

$$\zeta(\alpha) = \sum_{n=1}^{\infty} \frac{1}{n^\alpha}, \quad (\alpha > 1), \quad \zeta(\alpha) = \frac{1}{1 - 2^{1-\alpha}} \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n^\alpha}, \quad (\alpha > 0).$$

The Riemann zeta function is a special case ($x = 1$) of the *polylogarithm function* is defined as

$$Li_\alpha(x) = \sum_{n=1}^{\infty} \frac{x^n}{n^\alpha} = x + \frac{x^2}{2^\alpha} + \dots + \frac{x^n}{n^\alpha} + \dots$$

The polylogarithm function has properties

$$Li_\alpha(x) + Li_\alpha(-x) = 2^{1-\alpha} Li_\alpha(x^2), \quad (5)$$

$$Li_\alpha(x) = \Gamma(1 - \alpha) \left(\ln \frac{1}{x} \right)^{\alpha-1} + \sum_{n=0}^{\infty} \frac{\zeta(\alpha - n)}{n!} (\ln x)^n, \quad (6)$$

where $\alpha \neq 1, 2, 3, \dots$ and $|\ln x| < 2\pi$. From (6) with $x = e^{i\omega h}$ we obtain

$$\begin{aligned} Li_\alpha(e^{i\omega h}) &= \Gamma(1-\alpha)(-i\omega)^{\alpha-1}h^{\alpha-1} + \zeta(\alpha) - (-i\omega)\zeta(\alpha-1)h \\ &\quad + (-i\omega)^2 \frac{\zeta(\alpha-2)}{2}h^2 - (-i\omega)^3 \frac{\zeta(\alpha-3)}{6}h^3 + O(h^4). \end{aligned} \quad (7)$$

In [6] we use the Fourier transform method to derive the asymptotic expansion formula of the trapezoidal approximation for the fractional integral

$$\begin{aligned} h^\alpha \sum_{k=1}^{N-1} \frac{y(x-kh)}{k^{1-\alpha}} &= \int_0^x \frac{y(t)}{(x-t)^{1-\alpha}} dt + \sum_{k=0}^{\infty} (-1)^k \frac{\zeta(1-\alpha-k)}{k!} y^{(k)}(x) h^{k+\alpha} \\ &\quad - \Gamma(\alpha) \sum_{k=0}^{\infty} \frac{B_{k+1}}{(k+1)!} \left(\sum_{m=0}^k (-1)^m \binom{k}{m} \frac{x^{\alpha-m-1}}{\Gamma(\alpha-m)} y^{(m-k)}(0) \right) h^{k+1}. \end{aligned}$$

In the first part of this paper [7] we obtain approximations (8) and (9) for the Caputo derivative of order $2-\alpha$.

$$\frac{1}{2\Gamma(1-\alpha)h^\alpha} \sum_{k=0}^n \sigma_k^{(\alpha)} y_{n-k} = y_n^{(\alpha)} + O(h^{2-\alpha}), \quad (8)$$

where $\sigma_0^{(\alpha)} = 1 - 2\zeta(\alpha)$, $\sigma_1^{(\alpha)} = \frac{1}{2^\alpha} + 2\zeta(\alpha)$ and

$$\sigma_k^{(\alpha)} = \frac{1}{(k+1)^\alpha} - \frac{1}{(k-1)^\alpha}, \quad (k = 2, \dots, n-2),$$

$$\sigma_{n-1}^{(\alpha)} = -\frac{1}{(n-2)^\alpha} - 2 \left(\sum_{k=1}^{n-1} \frac{1}{k^\alpha} - \frac{n^{1-\alpha}}{1-\alpha} - \zeta(\alpha) \right),$$

$$\sigma_n^{(\alpha)} = -\frac{1}{(n-1)^\alpha} + 2 \left(\sum_{k=1}^{n-1} \frac{1}{k^\alpha} - \frac{n^{1-\alpha}}{1-\alpha} - \zeta(\alpha) \right).$$

$$\frac{1}{\Gamma(-\alpha)h^\alpha} \sum_{k=0}^n \sigma_k^{(\alpha)} y_{n-k} = y_n^{(\alpha)} + O(h^{2-\alpha}), \quad (9)$$

where $\sigma_0^{(\alpha)} = \zeta(\alpha) - \zeta(1+\alpha)$, $\sigma_1^{(\alpha)} = 1 - \zeta(\alpha)$ and

$$\sigma_k^{(\alpha)} = \frac{1}{k^{1+\alpha}}, \quad (k = 2, \dots, n-2),$$

$$\sigma_{n-1}^{(\alpha)} = \frac{1}{(n-1)^{1+\alpha}} - \frac{n^{1-\alpha}}{\alpha(1-\alpha)} + n \left(\zeta(1+\alpha) - \sum_{k=1}^{n-1} \frac{1}{k^{1+\alpha}} \right) - \left(\zeta(\alpha) - \sum_{k=1}^{n-1} \frac{1}{k^\alpha} \right),$$

$$\sigma_n^{(\alpha)} = (1-n) \left(\zeta(1+\alpha) - \sum_{k=1}^{n-1} \frac{1}{k^{1+\alpha}} \right) + \left(\zeta(\alpha) - \sum_{k=1}^{n-1} \frac{1}{k^\alpha} \right) + \frac{n^{1-\alpha}}{\alpha(1-\alpha)}.$$

In section 2 we use the Fourier transform method to derive the asymptotic expansion formula (18) of approximation (19). In section 3 we use (18) we obtain approximation (10) for the Caputo derivative of order $2 - \alpha$ and the second-order approximation (11).

$$\frac{1}{\Gamma(1-\alpha)h^\alpha} \sum_{k=0}^n \sigma_k^{(\alpha)} y_{n-k} = y_n^{(\alpha)} + O(h^{2-\alpha}), \quad (10)$$

where

$$\sigma_0^{(\alpha)} = 2^\alpha - (2^\alpha - 1)\zeta(\alpha), \quad \sigma_1^{(\alpha)} = \left(\frac{2}{3}\right)^\alpha - 2^\alpha + (2^\alpha - 1)\zeta(\alpha),$$

$$\sigma_k^{(\alpha)} = 2^\alpha \left(\frac{1}{(2k+1)^\alpha} - \frac{1}{(2k-1)^\alpha} \right), \quad (k = 2, \dots, n-2),$$

$$\sigma_{n-1}^{(\alpha)} = \frac{2^\alpha}{(2n-1)^\alpha} - \frac{2^\alpha}{(2n-3)^\alpha} + \frac{n^{1-\alpha}}{1-\alpha} - \zeta(\alpha) - 2^\alpha \left(\sum_{k=1}^n \frac{1}{(2k-1)^\alpha} - \zeta(\alpha) \right),$$

$$\sigma_n^{(\alpha)} = -\frac{2^\alpha}{(2n-1)^\alpha} + \zeta(\alpha) - \frac{n^{1-\alpha}}{1-\alpha} + 2^\alpha \left(\sum_{k=1}^n \frac{1}{(2k-1)^\alpha} - \zeta(\alpha) \right).$$

$$\frac{1}{\Gamma(1-\alpha)h^\alpha} \sum_{k=0}^n \delta_k^{(\alpha)} y_{n-k} = y_n^{(\alpha)} + O(h^2), \quad (11)$$

where $\delta_k^{(\alpha)} = \sigma_k^{(\alpha)}$, $(k = 3, \dots, n)$ and

$$\delta_0^{(\alpha)} = 2^\alpha + \frac{3}{2}(1-2^\alpha)\zeta(\alpha) + (2^{\alpha-1} - 1)\zeta(\alpha-1),$$

$$\delta_1^{(\alpha)} = 2^\alpha \left(\frac{1}{3^\alpha} - 1 \right) - 2(1-2^\alpha)\zeta(\alpha) - 2(2^{\alpha-1} - 1)\zeta(\alpha-1),$$

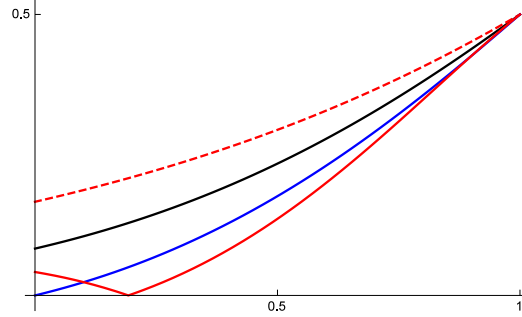
$$\delta_2^{(\alpha)} = 2^\alpha \left(\frac{1}{5^\alpha} - \frac{1}{3^\alpha} \right) + \frac{1}{2} (1 - 2^\alpha) \zeta(\alpha) + (2^{\alpha-1} - 1) \zeta(\alpha - 1).$$

The weights of the $L1$ approximation satisfy (2). Approximations (8),(9) and (10) have similar properties of the weights. These properties are used in the proofs for the convergence of the numerical solutions. An important factor for the accuracy of the numerical solutions of order $2 - \alpha$ which use approximations (1),(8),(9) and (10) for the Caputo derivative is the coefficient of the term $y''(x)h^{2-\alpha}$ in the asymptotic expansion formulas of the approximations. Approximations (1),(8),(9) and (10) have coefficients

$$C_1(\alpha) = \frac{\zeta(\alpha - 1)}{\Gamma(2 - \alpha)}, C_8(\alpha) = \frac{\zeta(\alpha) - 2\zeta(\alpha - 1)}{2\Gamma(1 - \alpha)}, C_9(\alpha) = \frac{\zeta(\alpha) - \zeta(\alpha - 1)}{2\Gamma(-\alpha)},$$

$$C_{10}(\alpha) = \frac{(2 - 2^\alpha) \zeta(\alpha - 1) - (2^\alpha - 1) \zeta(\alpha)}{2\Gamma(1 - \alpha)}.$$

Figure 1: Graph of the absolute value of the coefficients $C_1(\alpha)$ (black), $C_8(\alpha)$ (dashed), $C_9(\alpha)$ (blue) and $C_{10}(\alpha)$ (red) for $0 < \alpha < 1$.



In Figure 1 we compare the absolute values of the coefficients $C_1(\alpha)$, $C_8(\alpha)$, $C_9(\alpha)$ and $C_{10}(\alpha)$. In the first part of this paper [7] we derive approximations (8) and (9) for the Caputo derivative and we apply the approximations for computing the numerical solution of the fractional relaxation equation. The accuracy of the numerical solution of Equation I, Equation II and Equation III which uses approximation (9) is higher than the accuracy of the numerical solutions using (1) and (8). In Table 1 and Table 3 we compute the errors of the numerical solutions of Equation I, Equation II and Equation III which use approximations (1) and (10). The numerical solution which uses approximation (10) for the Caputo derivative has a higher

accuracy than the numerical solution using the $L1$ approximation (1). The improvement is 30% for Equation I and $\alpha = 0.25$, 15% for Equation II and $\alpha = 0.5$ and 4.7% for Equation III with $\alpha = 0.75$. In section 4 we construct a finite difference scheme for the fractional subdiffusion equation with accuracy $O(\tau^{2-\alpha} + h^2)$, using approximation (10) for the Caputo derivative and we analyse the convergence of the scheme.

2 Approximation for the Caputo Derivative of Order $4 - \alpha$

The construction of approximation (8) is based on the trapezoidal approximation for the fractional integral and the second-order backward difference approximation for the first derivative on each subinterval. The coefficient $C_8(\alpha)$ of the term $y_n'' h^{2-\alpha}$ in the expansion of approximation (8) is greater than the coefficient $C_1(\alpha)$ of the $L1$ approximation. The midpoint approximation for the definite integral is around twice more accurate than the trapezoidal approximation. In this section we use the Fourier transform method to derive approximations (10) and (11) for the Caputo derivative of order $2 - \alpha$ and 2 based on the midpoint approximation for the fractional integral. The coefficient $C_{10}(\alpha)$ of approximation (10) is smaller than $C_1(\alpha)$. The accuracy of the numerical solutions of Equation I, Equation II and Equation III which use approximation (10) for the Caputo derivative is higher than the accuracy of the numerical solutions which use the $L1$ approximation (1). The exponential Fourier Transform of the function y is defined as

$$\mathcal{F}[y(x)](w) = \hat{y}(w) = \int_{-\infty}^{\infty} e^{iwt} y(t) dt.$$

The Fourier transform has properties $\mathcal{F}[y(x - b)](w) = e^{iwb} \hat{y}(w)$ and

$$\mathcal{F}[D^\alpha y(x)](w) = (-iw)^\alpha \hat{y}(w), \quad \mathcal{F}[I^\alpha y(x)](w) = (-iw)^{-\alpha} \hat{y}(w).$$

From the midpoint approximation for the fractional integral in the definition of the Caputo derivative

$$y^{(\alpha)}(x) \approx \frac{h}{\Gamma(1-\alpha)} \sum_{k=1}^n \frac{y'(x_{k-1/2})}{(x - x_{k-1/2})^\alpha} = \frac{h^{1-\alpha}}{\Gamma(1-\alpha)} \sum_{k=1}^n \frac{y'_{k-1/2}}{(n - k + 1/2)^\alpha}.$$

By approximating $y'_{k-1/2} \approx (y_k - y_{k-1})/h$ we obtain

$$y^{(\alpha)}(x) \approx \frac{2^\alpha h^{1-\alpha}}{\Gamma(1-\alpha)} \sum_{k=1}^n \frac{y'_{k-1/2}}{(2n - 2k + 1)^\alpha} \approx \frac{2^\alpha}{\Gamma(1-\alpha) h^\alpha} \sum_{k=1}^n \frac{y_k - y_{k-1}}{(2n - 2k + 1)^\alpha}.$$

Substitute $K = n - k$

$$\Gamma(1-\alpha) \left(\frac{h}{2}\right)^\alpha y^{(\alpha)}(x) \approx \sum_{K=0}^{n-1} \frac{y_{n-K} - y_{n-K+1}}{(2K+1)^\alpha} = \sum_{k=0}^{n-1} \frac{y_{n-K}}{(2K+1)^\alpha} - \sum_{k=0}^{n-1} \frac{y_{n-K+1}}{(2K+1)^\alpha},$$

$$y^{(\alpha)}(x) \approx \frac{2^\alpha}{\Gamma(1-\alpha)h^\alpha} \left(\sum_{k=0}^{n-1} \frac{y_{n-k}}{(2k+1)^\alpha} - \sum_{k=1}^n \frac{y_{n-k}}{(2k-1)^\alpha} \right).$$

Denote

$$S_n[y] = \sum_{k=0}^{n-1} \frac{y_{n-k}}{(2k+1)^\alpha} - \sum_{k=1}^n \frac{y_{n-k}}{(2k-1)^\alpha}. \quad (12)$$

$$S_n[y] = y_n + \sum_{k=1}^{n-1} \left(\frac{1}{(2k+1)^\alpha} - \frac{1}{(2k-1)^\alpha} \right) y_{n-k} - \frac{y_0}{(2n-1)^\alpha}. \quad (13)$$

The generating function of an approximation is related to the Fourier transform of the approximation. The Fourier transform/generating function method is used by Ding and Li [8], Lubich [15], Tian et. al. [24] for constructing approximations for the fractional derivative. By applying Fourier transform to (12) and letting $n \rightarrow \infty$

$$\mathcal{F}[S_\infty[y]](w) = \left(\sum_{k=0}^{\infty} \frac{e^{iwkh}}{(2k+1)^\alpha} - \sum_{k=1}^{\infty} \frac{e^{iwkh}}{(2k-1)^\alpha} \right) \hat{y}(w).$$

Denote $W = e^{iwh/2}$.

$$\mathcal{F}[S_\infty[y]](w) = \left(\sum_{k=0}^{\infty} \frac{W^{2k}}{(2k+1)^\alpha} - \sum_{k=1}^{\infty} \frac{W^{2k}}{(2k-1)^\alpha} \right) \hat{y}(w),$$

$$\mathcal{F}[S_\infty[y]](w) = \hat{y}(w) \left(\frac{1}{W} - W \right) \sum_{k=1}^{\infty} \frac{W^{2k-1}}{(2k-1)^\alpha}.$$

From (5)

$$\begin{aligned} 2 \sum_{k=1}^{\infty} \frac{W^{2k-1}}{(2k-1)^\alpha} &= Li_\alpha(W) - Li_\alpha(-W) = 2Li_\alpha(W) - Li_\alpha(W) - Li_\alpha(-W) \\ &= 2Li_\alpha(W) - 2^{1-\alpha} Li_\alpha(W^2). \end{aligned}$$

Then

$$\mathcal{F}[S_\infty[y]](w) = \hat{y}(w) \left(e^{-\frac{iwh}{2}} - e^{\frac{iwh}{2}} \right) \left(Li_\alpha(e^{\frac{iwh}{2}}) - \frac{1}{2^\alpha} Li_\alpha(e^{iwh}) \right).$$

From the Taylor expansion formula of the exponential function

$$e^{-\frac{iwh}{2}} - e^{\frac{iwh}{2}} = (-iwh) + \frac{(-iwh)^3}{24} + O(h^5). \quad (14)$$

From (7) the function $Li_\alpha(e^{\frac{iwh}{2}})$ has fourth-order expansion

$$\begin{aligned} Li_\alpha(e^{\frac{iwh}{2}}) &= \frac{\Gamma(1-\alpha)}{2^{\alpha-1}} (-iwh)^{\alpha-1} + \zeta(\alpha) - (-iwh) \frac{\zeta(\alpha-1)}{2} h \\ &\quad + (-iwh)^2 \frac{\zeta(\alpha-2)}{8} h^2 - (-iwh)^3 \frac{\zeta(\alpha-3)}{48} h^3 + O(h^4). \end{aligned} \quad (15)$$

By combining (7) and (15) we obtain

$$\begin{aligned} Li_\alpha(e^{\frac{iwh}{2}}) - \frac{1}{2^\alpha} Li_\alpha(e^{iwh}) &= \frac{\Gamma(1-\alpha)}{2^\alpha} (-iwh)^{\alpha-1} h^{\alpha-1} + \left(1 - \frac{1}{2^\alpha}\right) \zeta(\alpha) \\ &\quad - (-iwh) \left(\frac{1}{2} - \frac{1}{2^\alpha}\right) \zeta(\alpha-1) h + (-iwh)^2 \frac{1}{2} \left(\frac{1}{4} - \frac{1}{2^\alpha}\right) \zeta(\alpha-2) h^2 \\ &\quad - (-iwh)^3 \frac{1}{6} \left(\frac{1}{8} - \frac{1}{2^\alpha}\right) \zeta(\alpha-3) h^3 + O(h^4). \end{aligned} \quad (16)$$

From (14) and (16)

$$\begin{aligned} \mathcal{F}[S_\infty[y]](w)/\hat{y}(w) &= \frac{\Gamma(1-\alpha)}{2^\alpha} (-iwh)^\alpha + (-iwh) \left(1 - \frac{1}{2^\alpha}\right) \zeta(\alpha) h \\ &\quad - (-iwh)^2 \left(\frac{1}{2} - \frac{1}{2^\alpha}\right) \zeta(\alpha-1) h^2 + \frac{\Gamma(1-\alpha)}{24 \cdot 2^\alpha} (-iwh)^{2+\alpha} \\ &\quad + (-iwh)^3 \left(\frac{1}{24} \left(1 - \frac{1}{2^\alpha}\right) + \frac{1}{2} \left(\frac{1}{4} - \frac{1}{2^\alpha}\right)\right) \zeta(\alpha-2) h^3 + O(h^4). \end{aligned}$$

By applying inverse Fourier transform we obtain the expansion formula

$$\begin{aligned} \left(\frac{2}{h}\right)^\alpha S_n[y] &= \Gamma(1-\alpha) y_n^{(\alpha)} + 2^\alpha \left(1 - \frac{1}{2^\alpha}\right) \zeta(\alpha) y_n' h^{1-\alpha} + O(h^{4-\alpha}) \\ &\quad - 2^\alpha \left(\frac{1}{2} - \frac{1}{2^\alpha}\right) \zeta(\alpha-1) y_n'' h^{2-\alpha} + \frac{\Gamma(1-\alpha)}{24} \frac{d^2}{dx^2} y_n^{(\alpha)} h^2 \\ &\quad + 2^\alpha \left(\frac{1}{24} \left(1 - \frac{1}{2^\alpha}\right) \zeta(\alpha) + \frac{1}{2} \left(\frac{1}{4} - \frac{1}{2^\alpha}\right) \zeta(\alpha-2)\right) y_n''' h^{3-\alpha}. \end{aligned} \quad (17)$$

Denote

$$\omega_0^{(\alpha)} = 2^\alpha, \quad \omega_k^{(\alpha)} = 2^\alpha \left(\frac{1}{(2k+1)^\alpha} - \frac{1}{(2k-1)^\alpha} \right), \quad \omega_n^{(\alpha)} = -\frac{2^\alpha}{(2n-1)^\alpha},$$

where $k = 1, \dots, n-1$. From (13)

$$\left(\frac{2}{h} \right)^\alpha \frac{S_n[y]}{\Gamma(1-\alpha)} = \frac{1}{\Gamma(1-\alpha)h^\alpha} \sum_{k=0}^n \omega_k^{(\alpha)} y_{n-k} \approx y_n^{(\alpha)}.$$

From (17) and the properties of the inverse Fourier transform we obtain the expansion formula of approximation (19) for the Caputo derivative.

Lemma 1. *Let $y(0) = y'(0) = y''(0) = 0$. Then*

$$\begin{aligned} \frac{1}{\Gamma(1-\alpha)h^\alpha} \sum_{k=0}^n \omega_k^{(\alpha)} y_{n-k} &= y_n^{(\alpha)} + \frac{1}{\Gamma(1-\alpha)} (2^\alpha - 1) \zeta(\alpha) y_n' h^{1-\alpha} + O(h^{4-\alpha}) \\ &\quad - \frac{1}{\Gamma(1-\alpha)} (2^{\alpha-1} - 1) \zeta(\alpha-1) y_n'' h^{2-\alpha} + \frac{1}{24} \frac{d^2}{dx^2} y_n^{(\alpha)} h^2 \\ &\quad + \frac{1}{\Gamma(1-\alpha)} \left(\frac{1}{24} (2^\alpha - 1) \zeta(\alpha) + \frac{1}{2} (2^{\alpha-2} - 1) \zeta(\alpha-2) \right) y_n''' h^{3-\alpha}. \end{aligned} \quad (18)$$

Corollary 2. *Approximation for the Caputo derivative of order $1-\alpha$.*

$$\mathcal{A}_n^\omega[y] = \frac{1}{\Gamma(1-\alpha)h^\alpha} \sum_{k=0}^n \omega_k^{(\alpha)} y_{n-k} = y_n^{(\alpha)} + O(h^{1-\alpha}). \quad (19)$$

The function $y(x) = 1$ has Caputo derivative $y^{(\alpha)}(x) = 0$. Approximation (19) satisfies $\mathcal{A}_n^\omega[1] = 0$, because $\sum_{k=0}^n \omega_k^{(\alpha)} = 0$. Denote by Equation I, Equation II and Equation III the fractional relaxation equations with exact solutions $y(x) = 1 + x + x^2 + x^3 + x^4$, $y(x) = e^x$ and $y(x) = \cos(2\pi x)$.

$$\begin{aligned} y^{(\alpha)}(x) + y(x) &= 1 + x + x^2 + x^3 + x^4 + \frac{x^{1-\alpha}}{\Gamma(2-\alpha)} \\ &\quad + \frac{2x^{2-\alpha}}{\Gamma(3-\alpha)} + \frac{6x^{3-\alpha}}{\Gamma(4-\alpha)} + \frac{24x^{4-\alpha}}{\Gamma(5-\alpha)}, \quad y(0) = 1. \end{aligned} \quad (\text{Equation I})$$

$$y^{(\alpha)}(x) + y(x) = e^x + x^{1-\alpha} E_{1,2-\alpha}(x), \quad y(0) = 1. \quad (\text{Equation II})$$

$$\begin{aligned} y^{(\alpha)}(x) + y(x) &= \cos(2\pi x) + i\pi x^{1-\alpha} (E_{1,2-\alpha}(2\pi i x) - E_{1,2-\alpha}(-2\pi i x)), \\ y(0) &= 1. \end{aligned} \quad (\text{Equation III})$$

Table 2: Error and order of numerical solution $NS[\omega]$ of Equation I and $\alpha = 0.25$, Equation II and $\alpha = 0.5$ and Equation III with $\alpha = 0.75$.

h	Equation I		Equation II		Equation III	
	Error	Order	Error	Order	Error	Order
0.003125	0.0074860	0.7535	0.0247219	0.5063	0.332392	0.2884
0.0015625	0.0044450	0.7520	0.0174267	0.5045	0.273326	0.2823
0.00078125	0.0026410	0.7511	0.0122952	0.5032	0.225573	0.2770
0.000390625	0.0015696	0.7506	0.0086803	0.5023	0.186736	0.2726

3 Approximations for the Caputo Derivative of Order $2 - \alpha$, 2

In the present section we use approximation (18) to obtain approximations for the Caputo derivative of order $2 - \alpha$ and 2 and we apply the approximations for computing the numerical solution of the fractional relaxation equation

$$y^{(\alpha)}(x) + y(x) = F(x), \quad y(0) = y_0. \quad (20)$$

In [5] we showed that

$$\bar{y}_1 = \frac{y(0) + \Gamma(2 - \alpha)h^\alpha F(h)}{1 + \Gamma(2 - \alpha)h^\alpha}$$

is a second order approximation for the value of the solution $y(h)$. Let

$$\frac{1}{\Gamma(1 - \alpha)h^\alpha} \sum_{k=0}^n \lambda_k^{(\alpha)} y_{n-k} \approx y_n^{(\alpha)}$$

be an approximation for the Caputo derivative. By approximating the Caputo derivative in equation (20) we obtain

$$\frac{1}{\Gamma(1 - \alpha)h^\alpha} \sum_{k=0}^n \lambda_k^{(\alpha)} y_{n-k} + y_n \approx F_n,$$

$$\left(\lambda_0^{(\alpha)} + \Gamma(1 - \alpha)h^\alpha \right) y_n + \sum_{k=1}^n \lambda_k^{(\alpha)} y_{n-k} \approx \Gamma(1 - \alpha)h^\alpha F_n.$$

Let u_n be an approximation for the value of the exact solution $y_n = y(x_n)$ of equation (20). The numbers u_n are computed with $u_0 = y(0)$, $u_1 = \bar{y}_1$ and

$$u_n = \frac{1}{\lambda_0^{(\alpha)} + \Gamma(1 - \alpha)h^\alpha} \left(\Gamma(1 - \alpha)h^\alpha F_n - \sum_{k=1}^n \lambda_k^{(\alpha)} u_{n-k} \right). \quad (NS[\lambda])$$

3.1 Approximation for the Caputo derivative of order $2 - \alpha$

By approximating y'_n in (18) with first order backward difference

$$y'_n = \frac{y_n - y_{n-1}}{h} - \frac{h}{2}y''_n + O(h^2)$$

we obtain the approximation for the Caputo derivative

$$\mathcal{A}_n^{\bar{\sigma}}[y] = \frac{1}{\Gamma(1-\alpha)h^\alpha} \sum_{k=0}^n \bar{\sigma}_k^{(\alpha)} y_{n-k} = y_n^{(\alpha)} + O(h^{2-\alpha}), \quad (21)$$

where $\bar{\sigma}_k^{(\alpha)} = \bar{\omega}_k^{(\alpha)}$ for $k = 2, \dots, n$ and

$$\bar{\sigma}_0^{(\alpha)} = \omega_0^{(\alpha)} - (2^\alpha - 1)\zeta(\alpha), \quad \bar{\sigma}_1^{(\alpha)} = \omega_1^{(\alpha)} + (2^\alpha - 1)\zeta(\alpha).$$

Approximation (21) has accuracy $O(h^{2-\alpha})$ when the function y satisfies $y(0) = y'(0) = 0$, and $\mathcal{A}_n^{\bar{\sigma}}[1] = 0$, because $\sum_{k=0}^n \bar{\sigma}_k^{(\alpha)} = 0$. Denote

$$W_n = \left(\zeta(\alpha) - \frac{n^{1-\alpha}}{1-\alpha} + 2^\alpha \left(\sum_{k=1}^n \frac{1}{(2k-1)^\alpha} - \zeta(\alpha) \right) \right).$$

Claim 3. *Let $y(x) = x$. Then*

$$\mathcal{A}_n^{\bar{\sigma}}[y] - y^{(\alpha)}(x) = \frac{h^{1-\alpha}W_n}{\Gamma(1-\alpha)}.$$

Proof.

$$\Gamma(1-\alpha)h^\alpha \mathcal{A}_n^{\bar{\sigma}}[x] = \sum_{k=0}^n \bar{\sigma}_k^{(\alpha)}(x - kh) = x \sum_{k=0}^n \bar{\sigma}_k^{(\alpha)} - h \sum_{k=0}^n k \bar{\sigma}_k^{(\alpha)} = -h \sum_{k=1}^n k \bar{\sigma}_k^{(\alpha)},$$

$$\frac{\Gamma(1-\alpha)}{h^{1-\alpha}} \mathcal{A}_n^{\bar{\sigma}}[x] = (1 - 2^\alpha) \zeta(\alpha) + 2^\alpha \sum_{k=1}^{n-1} \left(\frac{k}{(2k-1)^\alpha} - \frac{k}{(2k+1)^\alpha} \right) + \frac{2^\alpha n}{(2n-1)^\alpha},$$

$$\mathcal{A}_n^{\bar{\sigma}}[x] = \frac{h^{1-\alpha}}{\Gamma(1-\alpha)} \left((1 - 2^\alpha) \zeta(\alpha) + 2^\alpha \sum_{k=1}^n \frac{1}{(2k-1)^\alpha} \right). \quad (22)$$

The function $y(x) = x$ has fractional derivative

$$y^{(\alpha)}(x) = \frac{x^{1-\alpha}}{\Gamma(2-\alpha)} = \frac{n^{1-\alpha}h^{1-\alpha}}{(1-\alpha)\Gamma(1-\alpha)}. \quad (23)$$

The statement of Claim 3 follows from (22) and (23). \square

The function $y(x) = x^2$ has fractional derivative $y^{(\alpha)}(x) = x^{2-\alpha}/\Gamma(3-\alpha)$. Approximation (25) for the Caputo derivative has accuracy $O(h^{2-\alpha})$ for small values of n when $\mathcal{A}_n^\sigma[1] = 0$ and $\mathcal{A}_n^\sigma[x] = x^{1-\alpha}/\Gamma(2-\alpha)$. Represent the function $y(x)$ as

$$y(x) = y(x) - y(0) - y'(0)x + y(0) + y'(0)x = z(x) + y(0) + y'(0)x. \quad (24)$$

The function $z(x) = y(x) - y(0) - y'(0)x$ satisfies $z(0) = z'(0) = 0$. Then

$$\mathcal{A}_n^{\bar{\sigma}}[z(x)] = z^{(\alpha)}(x) + O(h^{2-\alpha}) = y^{(\alpha)}(x) - y'(0)\frac{x^{1-\alpha}}{\Gamma(2-\alpha)} + O(h^{2-\alpha}).$$

From (24)

$$\begin{aligned} \mathcal{A}_n^{\bar{\sigma}}[y(x)] &= \mathcal{A}_n^{\bar{\sigma}}[z(x)] + \mathcal{A}_n^{\bar{\sigma}}[y(0) + y'(0)x], \\ \mathcal{A}_n^{\bar{\sigma}}[y(x)] &= y^{(\alpha)}(x) - y'(0)\frac{x^{1-\alpha}}{\Gamma(2-\alpha)} + y'(0)\mathcal{A}_n^{\bar{\sigma}}[x] + O(h^{2-\alpha}). \end{aligned}$$

From Claim 3

$$\frac{1}{\Gamma(1-\alpha)h^\alpha} \sum_{k=0}^n \bar{\sigma}_k y_{n-k} = y_n^{(\alpha)} + \frac{y'(0)W_n h^{1-\alpha}}{\Gamma(1-\alpha)} + O(h^{2-\alpha}).$$

By approximating y'_0 with $y'_0 = (y_1 - y_0)/h + O(h)$ we obtain

$$\mathcal{A}_n^\sigma[y] = \frac{1}{\Gamma(1-\alpha)h^\alpha} \sum_{k=0}^n \sigma_k^{(\alpha)} y_{n-k} = y_n^{(\alpha)} + O(h^{2-\alpha}), \quad (25)$$

where $\sigma_k^{(\alpha)} = \bar{\sigma}_k^{(\alpha)}$ for $k = 0, \dots, n-2$ and

$$\sigma_{n-1}^{(\alpha)} = \bar{\sigma}_{n-1}^{(\alpha)} - W_n, \quad \sigma_n^{(\alpha)} = \bar{\sigma}_n^{(\alpha)} + W_n.$$

The weights $\sigma_k^{(\alpha)}$ of approximation (25) satisfy (2). When $n = 2$

$$\sigma_0^{(\alpha)} = 1 - 2\zeta(\alpha), \sigma_1^{(\alpha)} = 4\zeta(\alpha) + \frac{2^{2-\alpha}}{1-\alpha} - 2, \sigma_2^{(\alpha)} = -2\zeta(\alpha) - \frac{2^{2-\alpha}}{1-\alpha} + 1.$$

Table 3: Error and order of numerical solution $NS[\sigma]$ of Equation I and $\alpha = 0.25$, Equation II and $\alpha = 0.5$ and Equation III with $\alpha = 0.75$.

h	Equation I		Equation II		Equation III	
	Error	Order	Error	Order	Error	Order
0.003125	0.0000363	1.7152	0.0000453	1.4911	0.0023142	1.2460
0.0015625	0.0000110	1.7219	0.0000161	1.4940	0.0009744	1.2480
0.00078125	3.3×10^{-6}	1.7270	5.7×10^{-6}	1.4959	0.0004010	1.2489
0.000390625	1.0×10^{-6}	1.7310	2.0×10^{-6}	1.4972	0.0001724	1.2494

3.2 Second-Order Approximation for the Caputo derivative

By approximating y'_n and y''_n in (18) with

$$y'_n = \frac{1}{h} \left(\frac{3}{2} y_n - 2y_{n-1} + \frac{1}{2} y_{n-2} \right) + O(h^2),$$

$$y''_n = \frac{1}{h^2} (y_n - 2y_{n-1} + y_{n-2}) + O(h),$$

we obtain the approximation for the Caputo derivative

$$\frac{1}{\Gamma(1-\alpha)h^\alpha} \sum_{k=0}^n \bar{\delta}_k^{(\alpha)} y_{n-k} = y_n^{(\alpha)} + O(h^2), \quad (26)$$

where $\bar{\delta}_k^{(\alpha)} = \omega_k^{(\alpha)}$ for $k = 3, \dots, n$ and

$$\bar{\delta}_0^{(\alpha)} = \omega_0^{(\alpha)} + \frac{3}{2} (1 - 2^\alpha) \zeta(\alpha) + (2^{\alpha-1} - 1) \zeta(\alpha - 1),$$

$$\bar{\delta}_1^{(\alpha)} = \omega_1^{(\alpha)} - 2 (1 - 2^\alpha) \zeta(\alpha) - 2 (2^{\alpha-1} - 1) \zeta(\alpha - 1),$$

$$\bar{\delta}_2^{(\alpha)} = \omega_2^{(\alpha)} + \frac{1}{2} (1 - 2^\alpha) \zeta(\alpha) + (2^{\alpha-1} - 1) \zeta(\alpha - 1).$$

Approximation (26) has accuracy $O(h^2)$ when $y(0) = y'(0) = 0$. From approximation (26) we obtain the second order approximation approximation for the Caputo derivative

$$\frac{1}{\Gamma(1-\alpha)h^\alpha} \sum_{k=0}^n \delta_k^{(\alpha)} y_{n-k} = y_n^{(\alpha)} + O(h^2),$$

where $\delta_k^{(\alpha)} = \bar{\delta}_k^{(\alpha)}$ for $k = 0, 1, \dots, n-2$ and

$$\delta_{n-1}^{(\alpha)} = \bar{\delta}_{n-1}^{(\alpha)} - W_n, \quad \delta_n^{(\alpha)} = \bar{\delta}_n^{(\alpha)} + W_n.$$

The formulas for the weights $\delta_{n-1}^{(\alpha)}$ and $\delta_n^{(\alpha)}$ are derived using the method for computing the weights $\sigma_{n-1}^{(\alpha)}$ and $\sigma_n^{(\alpha)}$ from the previous section. In Figure 2 we compare numerical solutions $NS[\omega]$, $NS[\sigma]$ and $NS[\delta]$ of Equation III and $\alpha = 0.6$. In Table 4 we compute the error and the order of numerical solution $NS[\delta]$ of Equation I and $\alpha = 0.25$, Equation II and $\alpha = 0.5$ and Equation III with $\alpha = 0.75$.

Figure 2: Graph of the exact solution of Equation III and numerical solutions $NS[\omega]$ (green), $NS[\sigma]$ (red) and $NS[\delta]$ (blue) for $\alpha = 0.6, h = 0.1$.

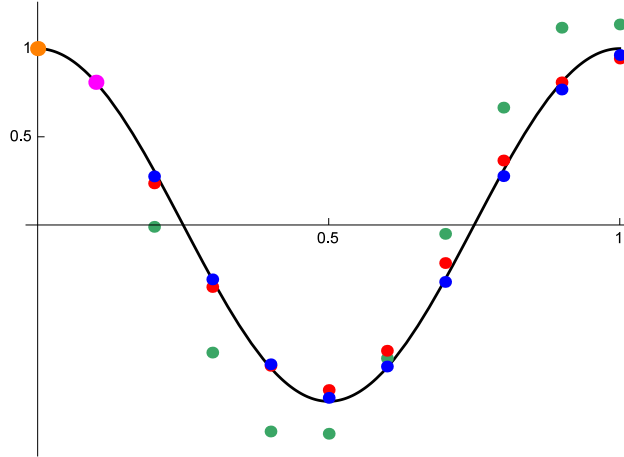


Table 4: Error and order of numerical solution $NS[\delta]$ of Equation I and $\alpha = 0.25$, Equation II and $\alpha = 0.5$ and Equation III with $\alpha = 0.75$.

h	Equation I		Equation II		Equation III	
	Error	Order	Error	Order	Error	Order
0.003125	4.2×10^{-6}	1.9602	1.6×10^{-6}	1.9748	0.00012247	1.9781
0.0015625	1.1×10^{-6}	1.9768	3.9×10^{-7}	1.9813	0.00003089	1.9874
0.00078125	2.7×10^{-7}	1.9864	9.9×10^{-8}	1.9863	7.8×10^{-6}	1.9926
0.000390625	6.8×10^{-8}	1.9919	2.5×10^{-8}	1.9901	1.9×10^{-6}	1.9956

4 Numerical Solution of the Fractional Subdiffusion Equation

The analytical and numerical solutions of the fractional subdiffusion equation have been studied extensively [5, 12, 14, 17, 18, 22, 28]. In this section we use approximation (10) for the Caputo derivative to construct a finite-difference scheme for the fractional subdiffusion equation

$$\begin{cases} \frac{\partial^\alpha u(x, t)}{\partial t^\alpha} = D \frac{\partial^2 u(x, t)}{\partial x^2} + F(x, t), & (x, t) \in [0, 1] \times [0, T], \\ u(x, 0) = u_0(x), \quad u(0, t) = u_L(t), \quad u(1, t) = u_R(t). \end{cases} \quad (27)$$

Let $h = 1/N, \tau = T/M$, where M and N are positive integers, and \mathcal{G} be a grid on the square $[0, 1] \times [0, T]$

$$\mathcal{G} = \{(nh, m\tau) | 1 \leq n \leq N, 1 \leq m \leq M\}.$$

Denote $u_n^m = u(nh, m\tau)$ and $F_n^m = F(nh, m\tau)$. By approximating the Caputo derivative in the time direction using (10) and the second derivative in the space direction by second-order central difference approximation we obtain

$$\frac{1}{\Gamma(1-\alpha)\tau^\alpha} \sum_{k=0}^n \sigma_k^{(\alpha)} u_n^{m-k} = D \frac{u_{n-1}^m - 2u_n^m + u_{n+1}^m}{h^2} + F_n^m + O(\tau^{2-\alpha} + h^2).$$

Let $\eta = \Gamma(1-\alpha)D\tau^\alpha/h^2$. The numerical solution $\{U_n^m\}_{n=1}^{N-1}$ of equation (27) satisfies the system of equations

$$-\eta U_{n-1}^m + \left(\sigma_0^{(\alpha)} + 2\eta\right) U_n^m - \eta U_{n+1}^m = -\sum_{k=1}^n \sigma_k^{(\alpha)} U_n^{m-k} + \tau^\alpha \Gamma(1-\alpha) F_n^m.$$

Let \mathcal{K} be a tridiagonal matrix of dimension $N-1$ with values $\sigma_0^{(\alpha)} + 2\eta$ on the main diagonal, and $-\eta$ on the diagonals above and below the main diagonal. The vector $\mathcal{U}^m = (U_1^m, U_2^m, \dots, U_{N-1}^m)^T$ of the numerical solution on the m -th layer of the grid \mathcal{G} is a solution of the linear system

$$\mathcal{K}\mathcal{U}^m = \mathcal{R}_1 + \eta\mathcal{R}_2, \quad (28)$$

where \mathcal{R}_1 and \mathcal{R}_2 are the column vectors of dimension $N-1$

$$\mathcal{R}_1^T = \left[-\sum_{k=1}^n \sigma_k^{(\alpha)} U_n^{m-k} + \Gamma(1-\alpha)\tau^\alpha F(nh, m\tau) \right]_{n=1}^{N-1},$$

$$\mathcal{R}_2^T = [u_L(m\tau), 0, \dots, 0, u_R(m\tau)]^T.$$

The numerical solution of the fractional subdiffusion equation on the first layer of the grid \mathcal{G} is computed with the approximation [5]

$$y^{(\alpha)}(\tau) = \frac{y(\tau) - y(0)}{\tau^\alpha \Gamma(2 - \alpha)} + O(\tau^{2-\alpha}). \quad (29)$$

Let $\tilde{\eta} = \Gamma(2 - \alpha)D\tau^\alpha/h^2$. The numerical solution on the first layer of the grid \mathcal{G} satisfies the system of equations

$$\begin{cases} U_0^1 = u_L(\tau), U_N^1 = u_R(\tau), & (n = 1 \dots, N - 1), \\ -\tilde{\eta}U_{n-1}^1 + (1 + 2\tilde{\eta})U_n^1 - \tilde{\eta}U_{n+1}^1 = U_n^0 + \Gamma(2 - \alpha)\tau^\alpha F_n^1. \end{cases}$$

Example 1: The fractional subdiffusion equation

$$\begin{cases} \frac{\partial^\alpha v(x, t)}{\partial t^\alpha} = \frac{\partial^2 v(x, t)}{\partial x^2} + e^x (t^{1-\alpha} E_{1, 2-\alpha}(t) - e^t), \\ u(x, 0) = e^x, \quad u(0, t) = e^t, \quad u(1, t) = e^{t+1}, \quad (x, t) \in [0, 1] \times [0, 1], \end{cases} \quad (30)$$

has the solution $u(x, t) = e^{x+t}$.

Table 5: Maximum error and order of numerical solution (28) of the fractional subdiffusion equation (30) for $\alpha = 0.25, \alpha = 0.5, \alpha = 0.75$ at time $t = 1$.

h	$\alpha = 0.25$		$\alpha = 0.5$		$\alpha = 0.75$	
	<i>Error</i>	<i>Order</i>	<i>Error</i>	<i>Order</i>	<i>Error</i>	<i>Order</i>
0.025	0.00009999	1.7795	0.00043077	1.5094	0.00174603	1.2485
0.0125	0.00002917	1.7773	0.00015142	1.5084	0.00073415	1.2499
0.00625	8.5×10^{-6}	1.7742	0.00005328	1.5067	0.00030862	1.2503
0.003125	2.5×10^{-6}	1.7712	0.00001877	1.5053	0.00012972	1.2504

Example 2: The fractional subdiffusion equation

$$\begin{cases} \frac{\partial^\alpha u(x, t)}{\partial t^\alpha} = \frac{1}{\pi^2} \frac{\partial^2 u(x, t)}{\partial x^2}, & (x, t) \in [0, 1] \times [0, 1], \\ u(x, 0) = \sin(\pi x), \quad u(0, t) = 0, \quad u(1, t) = 0, \end{cases} \quad (31)$$

has the solution $u(x, t) = \sin(\pi x)E_\alpha(-t^\alpha)$. The first partial derivative of the solution is unbounded at $t = 0$.

Table 6: Maximum error and order of numerical solution (28) of the fractional subdiffusion equation (31) for $\alpha = 0.25, \alpha = 0.5, \alpha = 0.75$ at time $t = 1$.

h	$\alpha = 0.25$		$\alpha = 0.5$		$\alpha = 0.75$	
	<i>Error</i>	<i>Order</i>	<i>Error</i>	<i>Order</i>	<i>Error</i>	<i>Order</i>
0.025	0.00088407	1.2153	0.00185912	1.1413	0.00343405	1.1007
0.0125	0.00040631	1.1216	0.00087831	1.0818	0.00164008	1.0661
0.00625	0.00019418	1.0652	0.00042506	1.0471	0.00079469	1.0453
0.003125	0.00009483	1.0339	0.00020854	1.0274	0.00038844	1.0327

In Table 6 we compute the error and the order of numerical solution (28) for equation (31). The numerical results from Table 6 suggest that the accuracy of numerical solution (28) is $O(h)$. A numerical analysis of the scheme using the $L1$ approximation for the Caputo derivative is given by Jin, Lazarov and Zhou [14]. We use the fractional Taylor polynomials of the solution in order to improve the differentiability class of the solution and the accuracy of the numerical solution. Denote by $D_t^{[\beta]}u(x, t)$ the Miller-Ross derivative of order β of the solution $u(x, t)$ in the time direction. From equation (31)

$$D_t^{[\alpha]}u(x, t) = \frac{1}{\pi^2} \frac{\partial^2 u(x, t)}{\partial x^2}.$$

By applying fractional differentiation of order α we obtain

$$D_t^{[2\alpha]}u(x, t) = D_t^\alpha D_t^\alpha u(x, t) = \frac{1}{\pi^2} D_t^\alpha \frac{\partial^2 u(x, t)}{\partial x^2} = \frac{1}{\pi^4} \frac{\partial^4 u(x, t)}{\partial x^4},$$

$$D_t^{[3\alpha]}u(x, t) = D_t^\alpha D_t^{[2\alpha]}u(x, t) = \frac{1}{\pi^4} D_t^\alpha \frac{\partial^4 u(x, t)}{\partial x^4} = \frac{1}{\pi^6} \frac{\partial^6 u(x, t)}{\partial x^6}.$$

By induction we obtain

$$D_t^{[n\alpha]}u(x, t) = \frac{1}{\pi^{2n}} \frac{\partial^{2n} u(x, t)}{\partial x^{2n}}.$$

Set $t = 0$

$$D_t^{[n\alpha]}u(x, 0) = \frac{1}{\pi^{2n}} \frac{\partial^{2n} u(x, 0)}{\partial x^{2n}} = \frac{1}{\pi^{2n}} \frac{\partial^{2n} \sin x}{\partial x^{2n}} = (-1)^n \sin(\pi x).$$

The solution of the fractional subdiffusion equation (31) has fractional Taylor polynomials in the time direction

$$T_m^{(\alpha)}(x, t) = \sum_{n=0}^m \frac{t^{n\alpha} D_t^{[n\alpha]} u(x, 0)}{\Gamma(n\alpha + 1)} = \sin(\pi x) \sum_{n=0}^m (-1)^n \frac{h^{n\alpha}}{\Gamma(n\alpha + 1)}.$$

Substitute

$$v(x, t) = u(x, t) - \sin(\pi x) \sum_{n=0}^m (-1)^n \frac{t^{n\alpha}}{\Gamma(n\alpha + 1)}.$$

By differentiating $v(x, t)$ we obtain

$$D_t^\alpha v(x, t) = D_t^\alpha u(x, t) + \sin(\pi x) \sum_{n=0}^{m-1} (-1)^{n+1} \frac{t^{n\alpha}}{\Gamma(n\alpha + 1)},$$

$$\frac{\partial^2}{\partial x^2} v(x, t) = \frac{\partial^2}{\partial x^2} u(x, t) + \pi^2 \sin(\pi x) \sum_{n=0}^m (-1)^{n+1} \frac{t^{n\alpha}}{\Gamma(n\alpha + 1)}.$$

The function $v(x, t)$ is a solution of the fractional subdiffusion equation

$$\begin{cases} \frac{\partial^\alpha v(x, t)}{\partial t^\alpha} = \frac{1}{\pi^2} \frac{\partial^2 v(x, t)}{\partial x^2} + (-1)^{m+1} \sin(\pi x) \frac{t^{m\alpha}}{\Gamma(m\alpha + 1)}, \\ v(x, 0) = v(0, t) = v(\pi, t) = 0. \end{cases} \quad (32)$$

The solution $v(x, t)$ of equation (32) has a continuous second partial derivative in the time direction at the point $t = 0$, when $m\alpha \geq 2$. In Table 7 we compute the error and the order of numerical solution (28) of equation (32) and $\alpha = 0.25, 0.5, 0.75$. The accuracy of numerical solution (28) of equation (32) is $O(h^{2-\alpha})$ and the error is significantly smaller than the error of the numerical solution (28) of equation (31) in Table 6.

In Theorem 5 we establish the convergence of numerical solution (28) of the fractional subdiffusion equation. The proof uses estimate (34) for $\sigma_m^{(\alpha)}$.

Claim 4.

$$W_m = \frac{\alpha}{24m^{1+\alpha}} + O\left(\frac{1}{m^{2+\alpha}}\right).$$

Table 7: Maximum error and order of numerical solution (28) of the fractional subdiffusion equation (32) for $\alpha = 0.25$ and $m = 8$, $\alpha = 0.5$ and $m = 4$ and $\alpha = 0.75$, $m = 2$ at time $t = 1$.

h	$\alpha = 0.25$		$\alpha = 0.5$		$\alpha = 0.75$	
	<i>Error</i>	<i>Order</i>	<i>Error</i>	<i>Order</i>	<i>Error</i>	<i>Order</i>
0.025	0.00009044	1.8754	0.00027114	1.5611	0.00113616	1.2815
0.0125	0.00002484	1.8641	0.00009292	1.5449	0.00047144	1.2690
0.00625	6.9×10^{-6}	1.8534	0.00003212	1.5328	0.00019664	1.2615
0.003125	1.9×10^{-6}	1.8431	0.00001117	1.5238	0.00008228	1.2570

Proof. Denote $S_m = \sum_{k=1}^m 1/k^\alpha$. From the formula for the sum of powers

$$S_{m-1} = \zeta(\alpha) + \frac{m^{1-\alpha}}{1-\alpha} \sum_{n=0}^{\infty} \binom{1-\alpha}{m} \frac{B_m}{n^m},$$

$$S_m = \zeta(\alpha) + \frac{m^{1-\alpha}}{1-\alpha} + \frac{1}{2m^\alpha} - \frac{\alpha}{12m^{1+\alpha}} + O\left(\frac{1}{m^{2+\alpha}}\right). \quad (33)$$

We have that

$$S_{2m} = \sum_{k=1}^{2m} 1/k^\alpha = \sum_{k=1}^m \frac{1}{(2k-1)^\alpha} + \sum_{k=1}^m \frac{1}{(2k)^\alpha} = \sum_{k=1}^m \frac{1}{(2k-1)^\alpha} + \frac{1}{2^\alpha} S_m.$$

From (33)

$$S_{2m} - \frac{1}{2^\alpha} S_m = \zeta(\alpha) \left(1 - \frac{1}{2^\alpha}\right) + \frac{m^{1-\alpha}}{(1-\alpha)2^\alpha} + \frac{\alpha}{12(2m)^{1+\alpha}} + O\left(\frac{1}{m^{2+\alpha}}\right).$$

Hence

$$W_m = \zeta(\alpha) - \frac{m^{1-\alpha}}{1-\alpha} + 2^\alpha \left(S_{2m} - \frac{1}{2^\alpha} S_m - \zeta(\alpha)\right) = \frac{\alpha}{24m^{1+\alpha}} + O\left(\frac{1}{m^{2+\alpha}}\right).$$

□

We can further show that $W_m < \alpha / (24m^{1+\alpha})$. From Claim 4 we obtain

$$|\sigma_m^{(\alpha)}| > \frac{2^\alpha}{(2m-1)^\alpha} - W_m > \frac{1}{m^\alpha} - \frac{\alpha}{24m^{1+\alpha}} > \frac{23}{24m^\alpha} > \frac{1}{2m^\alpha}. \quad (34)$$

The maximum (infinity) norm of the vector $\mathcal{V} = (v_i)$ and the square matrix $\mathcal{L} = (l_{ij})$ of dimension $N - 1$ are defined as

$$\|\mathcal{V}\| = \max_{1 \leq i \leq N-1} |v_i|, \quad \|\mathcal{L}\| = \max_{1 \leq j \leq N-1} \sum_{m=1}^{N-1} |l_{mj}|.$$

The matrix \mathcal{K} is a diagonally dominant tridiagonal matrix with positive elements on the main diagonal and negative elements on the diagonals below and above the main diagonal. The matrix \mathcal{K}^{-1} is a positive matrix. From the Ahlberg-Nilson-Varah bound [2, 25]

$$\|\mathcal{K}^{-1}\| \leq \frac{1}{\sigma_0^{(\alpha)}}.$$

The numbers $\sigma_k^{(\alpha)}$ satisfy $\sum_{k=1}^m \left| \sigma_k^{(\alpha)} \right| = \sigma_0^{(\alpha)}$. From (34)

$$\sum_{k=1}^{m-1} \left| \sigma_k^{(\alpha)} \right| = \sigma_0^{(\alpha)} - \left| \sigma_m^{(\alpha)} \right| < \sigma_0^{(\alpha)} - \frac{1}{2m^\alpha}. \quad (35)$$

Let $e_n^m = u_n^m - U_n^m$ be the error of numerical solution (28). The error vector $\mathcal{E}^m = (e_n^m)$ on the m -th layer of the grid \mathcal{G} satisfies the system of equations

$$\mathcal{K}\mathcal{E}^m = \mathcal{R}^m,$$

where $\mathcal{R}^m = (r_n^m)$ is an $N - 1$ dimensional column vector with elements

$$r_n^m = - \sum_{k=1}^{m-1} \sigma_k^{(\alpha)} e_n^{m-k} + \tau^\alpha (A_n^m \tau^{2-\alpha} + B_n^m h^2),$$

and $A_n^m \tau^{2-\alpha} + B_n^m h^2$ is the approximation error at the point $(nh, m\tau)$. Let A be a positive constant such that $|A_n^m| < A$ and $|B_n^m| < A$, for all m and n . The numerical solution on the first layer of \mathcal{G} is computed using approximation (29), which is obtained from the the $L1$ approximation when $n = 1$. The convergence of the numerical solution of the time-fractional subdiffusion equation which uses the $L1$ approximation for the Caputo derivative is studied in [17, 18]. We can assume that the number A is large enough, such that (36) holds for $m = 1$.

Theorem 5. *The error on the m -th layer of the grid \mathcal{G} satisfies*

$$\|\mathcal{E}^m\| \leq 2Am^\alpha \tau^\alpha (\tau^{2-\alpha} + h^2). \quad (36)$$

Proof. Induction on m . Suppose that (36) holds for $k = 1, \dots, m-1$.

$$|r_n^m| \leq \sum_{k=1}^{m-1} \left| \sigma_k^{(\alpha)} \right| |e_n^{m-k}| + A\tau^\alpha (\tau^{2-\alpha} + h^2).$$

From the induction assumption and (35)

$$|r_n^m| \leq 2Am^\alpha \tau^\alpha (\tau^{2-\alpha} + h^2) \sum_{k=1}^{m-1} \left| \sigma_k^{(\alpha)} \right| + A\tau^\alpha (\tau^{2-\alpha} + h^2),$$

$$|r_n^m| \leq 2Am^\alpha \tau^\alpha (\tau^{2-\alpha} + h^2) \left(\sigma_0^{(\alpha)} - \frac{1}{2m^\alpha} \right) + A\tau^\alpha (\tau^{2-\alpha} + h^2),$$

$$|r_n^m| \leq 2A\sigma_0^{(\alpha)} m^\alpha \tau^\alpha (\tau^{2-\alpha} + h^2),$$

for all $n = 1, \dots, N-1$. Then

$$\|\mathcal{R}^m\| \leq 2A\sigma_0^{(\alpha)} m^\alpha \tau^\alpha (\tau^{2-\alpha} + h^2).$$

We have that $\mathcal{E}^m = \mathcal{K}^{-1}\mathcal{R}^m$. Hence

$$\|\mathcal{E}^m\| \leq \|\mathcal{K}^{-1}\| \|\mathcal{R}^m\| \leq \frac{1}{\sigma_0^{(\alpha)}} \|\mathcal{R}^m\| \leq 2Am^\alpha \tau^\alpha (\tau^{2-\alpha} + h^2).$$

□

From (36) we obtain the estimate for the error on the grid \mathcal{G}

$$\|\mathcal{E}^m\| \leq 2AM^\alpha \tau^\alpha (\tau^{2-\alpha} + h^2) \leq 2AT^\alpha (\tau^{2-\alpha} + h^2),$$

for all $m = 1, 2, \dots, M$.

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